CREST 3.0.1

Webpage

https://github.com/crest-lab/crest
https://crest-lab.github.io/crest-docs/

Version

3.0.1

Build Environment

- Intel oneAPI Compiler 2024.1.0 (icx and ifort)
- MKL 2024.1

Files Required

(Some files will be downloaded in the build procedure below.)

Build Procedure

```sh
#!/bin/sh

VERSION=3.0.1
INSTALL_PREFIX=/apl/crest/3.0.1

CREST_GITHUB=https://github.com/crest-lab/crest.git

WORKDIR=/gwork/users/${USER}

PARALLEL=24
export LANG=C

#-------------------------------------------------------------------
umask 0022

module -s purge

. ~/intel/oneapi/compiler/latest/env/vars.sh # 2024.1.0

module -s load mkl/2024.1

cd ${WORKDIR}
if [ -d crest ]; then
 mv crest crest_erase
 rm -rf crest_erase &
fi

export FC=ifort
export CC=icx

git clone ${CREST_GITHUB} -b v${VERSION}
cd crest

sed -i -e "s/-align array64byte//" config/CMakeLists.txt

mkdir build && cd build
cmake .. -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX}

make -j${PARALLEL}
make test
make install

cd ../
cp -r examples ${INSTALL_PREFIX}
```

Tests

All the tests have passed successfully.

Notes

- For some input, a flood of "Intel MKL ERROR: Parameter 6 was incorrect on entry to DLASWP." messages are shown if MKL 2023.1.0 (static or dynamic) is employed.
  - See https://github.com/crest-lab/crest/issues/285.
  - These messages are not shown if MKL 2023.2.0 or 2024.1.0 is employed. This issue seems to be specific to MKL 2023.1.0.
  - Precompiled binary releases (version 3.0.1, continuous release (May 7, 2024)) are also affected by this issue?
- QCG example job (https://crest-lab.github.io/crest-docs/page/examples/qcg/example_2.html) failed in the later part of the calculation when crest 3.0.1 is built with Intel compiler and CMake.
  - The error message is the same as that in this comment in https://github.com/crest-lab/crest/issues/278.
  - The option "-align array64byte", which is automatically added in CMake build, causes this error. The problem disappears when this option is removed (like the procedure above). This option may not be used for meson build.
- We couldn't use Intel 2024.1.0 with meson. (2023.1.0 is ok.)
  - (export FC="ifort -diag-disable=10448" was necessary in our try with meson and intel 2023.1.0)